Stat 471: Lecture 21
MCMC I.

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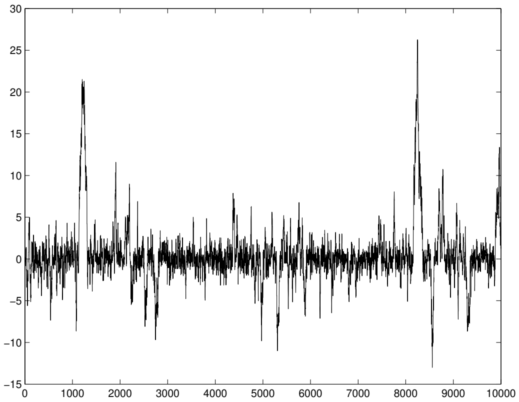

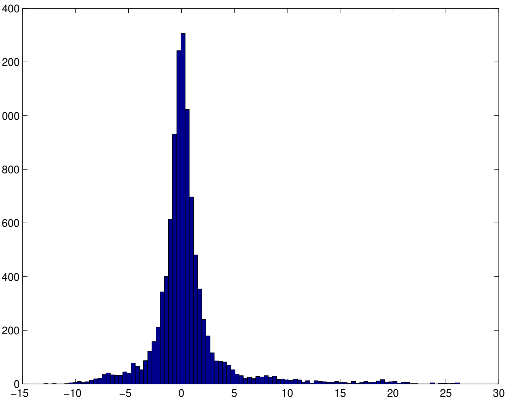

1. A *Markov chain Monte-Carlo* (MCMC) method for the simulation of a distribution π is any method producing a Markov chain X_i whose invariant distribution is π.

2. *Metropolis-Hastings Algorithm* (M-H). For given distribution π and conditional density $q(y|x)$ called *instrumental* or *proposal* distribution, define
$$\alpha(x,y) = \min\Big(\frac{\pi(y)}{\pi(x)}\frac{q(x|y)}{q(y|x)}, 1\Big).$$
Then we generate Markov chain X_i by
1. Initialize chain X_0 and $i = 0$.
2. Generate $Y \sim q(y|X_i)$.
3. Generate $U \sim Unif(0,1)$.
4. If $U \leq \alpha(X_i, Y)$, $X_{i+1} = Y$
else $X_{i+1} = X_i$.
5. Set $i = i + 1$ and goto step 2.
Note that $0 \leq \alpha(X_i, Y) \leq 1$ so the step 4 is equivalent to take $X_{i+1} = Y$ with probability $\alpha(X_i, Y)$ and $X_{i+1} = X_i$ with probability $1 - \alpha(X_i, Y)$. q should be easy to simulate from to be able to use M-H algorithm.

3. The transition kernel of the resulting chain X_i is $p_{xy} = q(y|x)\alpha(x,y)$ if $y \neq x$ and $p_{xx} = 1 - \sum_{u \neq x} p_{xu} = 1 - \sum_{u \neq x} q(u|x)\alpha(x,u)$. In this case it is trivial to show that
$$\pi(x)p_{xy} = \pi(y)p_{yx} \text{ (HW 4).}$$
This is called the *detailed balance condition* of a Markov chain. Then it can be shown that π is the invariant distribution and the chain is reversible, i.e. $p_{xy} = p_{yx}$.
Proof. $\sum_{y \in S} \pi(y)p_{yx} = \sum_{y \in S} \pi(x)p_{xy} = \pi(x)$. From Lecture 20, this is equivalent to the invariant condition in matrix form $\pi' = \pi'\mathbf{P}$.

4. The stationary of π is established for any conditional distribution q. This shows the universality of M-H algorithm. Based on M-H algorithm and the ergodic theorem, then we can estimate $\mathbb{E}_\pi g \approx \frac{1}{n-m}\sum_{i=m+1}^{n} g(X_i)$, where the initial chain X_0 and the conditional distribution q do not really matter.

5. For large m, $X_m, X_{m+1}, \cdots$ produces a dependent sample distributed from π (see Lecture 20 for detail). Let's generate 10000 Cauchy numbers from normal distribution using MCMC. Note that they will not be independent. Let $\pi(x) = \frac{1}{1+x^2}$ (no need to specify the normalizing constant) and $q(y|x) \sim N(x, 1)$

```
n=10000;
x(1)=0;
str=’exp(-(x-mu)^2/2)’;
snrpdf=inline(str,’x’,’mu’);
cauchypdf=inline(’1/(1+x^2)’);
for i=2:n
  y=x(i-1) + snrnd(1);
  alpha=min([1,snrpdf(y)/snrpdf(x(i-1))
  *snrpdf((x(i-1),y)/snrpdf(y,x(i-1))]);
  u=rand;
  if u <= alpha
    x(i)=y;
  else
    x(i)=x(i-1);
  end
end
```